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# Molecular data and radiative transfer tools for ALMA

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**Abstract** This paper presents an overview of several modeling tools for analyzing molecular line observations at sub-millimeter wavelengths. These tools are already proving to be very valuable for the interpretation of data from current telescopes, and will be indispensable for data obtained with ALMA. The tools are: (1) the Leiden Atomic and Molecular Database (LAMDA), a collection of spectroscopic data and collisional excitation rates; (2) RADEX, an on-line and off-line program to calculate non-LTE excitation and emission from a homogeneous medium, based on the escape probability approximation; (3) RATRAN, an accelerated Monte Carlo program to solve molecular excitation and radiative transfer in spherical and cylindrical symmetry. The paper presents examples of how to use these tools in conjunction with existing data reduction packages to quantitatively interpret submillimeter single-dish and interferometric observations. The described tools are publically available at

<http://www.strw.leidenuniv.nl/~moldata>.

The paper concludes with a discussion of future needs in the fields of molecular data and radiative transfer.

**Keywords** Radiative transfer · Methods: numerical · Submillimeter · Molecular data · Astronomical data bases

## 1 Introduction

Observations of spectral lines at radio, (sub)millimeter and infrared wavelengths are powerful tools to investigate the physical and chemical conditions in the dilute gas of astronomical sources where thermodynamic equilibrium is a poor approximation (Genzel 1991; Black 2000). To extract astrophysical parameters from the data, the excitation and optical depth of the lines need to be estimated, for which various methods may be used, depending on the available observations (Van Dishoeck & Hogerheijde 1999; Van der Tak 2005).

With the advent of ALMA, the need for efficient molecular line modeling tools will become more pressing than ever. This paper presents several such tools which we have developed and which we expect will become quite important for the analysis of ALMA data.

## 2 LAMDA

The Leiden Atomic and Molecular Database (LAMDA) (Schöier et al. 2005) contains spectroscopic and collisional data for 24 species of astrophysical interest. Most of these species are molecules, but data files for the fine structure lines of C, O and C<sup>+</sup> are also provided. The data files contain energy levels, statistical weights, Einstein A-coefficients and collisional rate coefficients. Available collisional data from quantum chemical calculations and experiments have been extrapolated to higher energies (up to  $E/k \sim 1000$  K). The format of the data files is such that they can be read directly into RADEX and RATRAN.

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### 3 RADEX

*Description* RADEX (Van der Tak et al. 2007) is a computer program to calculate the intensities of atomic and molecular lines produced in a uniform medium, based on statistical equilibrium calculations involving collisional and radiative processes. The treatment includes radiation from background sources; optical depth effects are calculated using the escape probability approximation. The user has a choice of geometries: uniform sphere, expanding sphere, or plane-parallel slab. The expanding sphere solution is analogous to the well-known LVG method.

*Availability* The program is available both as an on-line calculator for quick estimates and as an off-line package for detailed analysis of multi-line datasets.

*Typical Uses* (1) Multi-line observations of a region are available, and an estimate is needed of the average temperature, density, and column density. (2) Based on estimates of the typical conditions in a source, estimates are made of the expected line intensities, for example to prepare an observing proposal.

*Example* Ratios of submillimeter lines of HCN and  $\text{HCO}^+$  trace densities between  $10^3$  and  $10^8 \text{ cm}^{-3}$  and temperatures between 20 and 200 K. By observing 3–4 different transitions, density and temperature can be found (Fig. 1).

### 4 RATRAN

*Description* RATRAN (Hogerheijde & van der Tak 2000) is a computer program to simulate non-LTE line radiative transfer in spherical or cylindrical symmetry. The program uses the accelerated Monte Carlo method to represent the radiation field, which offers both speed and reliability.

Within these geometries, the source model can have any density, temperature, abundance, and velocity distribution. The program produces synthetic spectral line cubes for a given source distance and orientation. Third-party software such as Miriad or IDL readily produce higher-level output such as beam-convolved line fluxes or even simulated interferometric visibilities.

*Availability* The spherically symmetric version of the program is available as an off-line package. The cylindrically symmetric version is available on a collaborative basis.

*Typical Use* The user has obtained molecular line observations of an object, and wishes to quantitatively test a particular model. With RATRAN, he produces synthetic data and compares these to the observations by eye, or uses a  $\chi^2$  minimization to arrive at an optimum fit.

*Example* Brinch et al. (2007) compare observations of the Young Stellar Object L 1489 IRS to a model with infalling and rotational motions. The data set consists of millimeter interferometric observations, near-infrared scattered light imaging, and CO ro-vibrational lines. Comparison of data and model uses a Voronoi optimisation algorithm.

### 5 Future molecular data needs

Of the 134 molecules which are known in space, collisional rate coefficients (CRCs) exist only for twenty-four (§ 2). Accurate CRCs are important for reliable estimates of molecular column densities, and essential to estimate other parameters such as kinetic temperature and volume density. Recently several important molecules for which only inaccurate CRCs were known, based on outdated, low-quality potential energy surfaces, have been re-calculated, such as CS,  $\text{HC}_3\text{N}$ , and  $\text{CH}_3\text{OH}$  (Dubernet 2005).

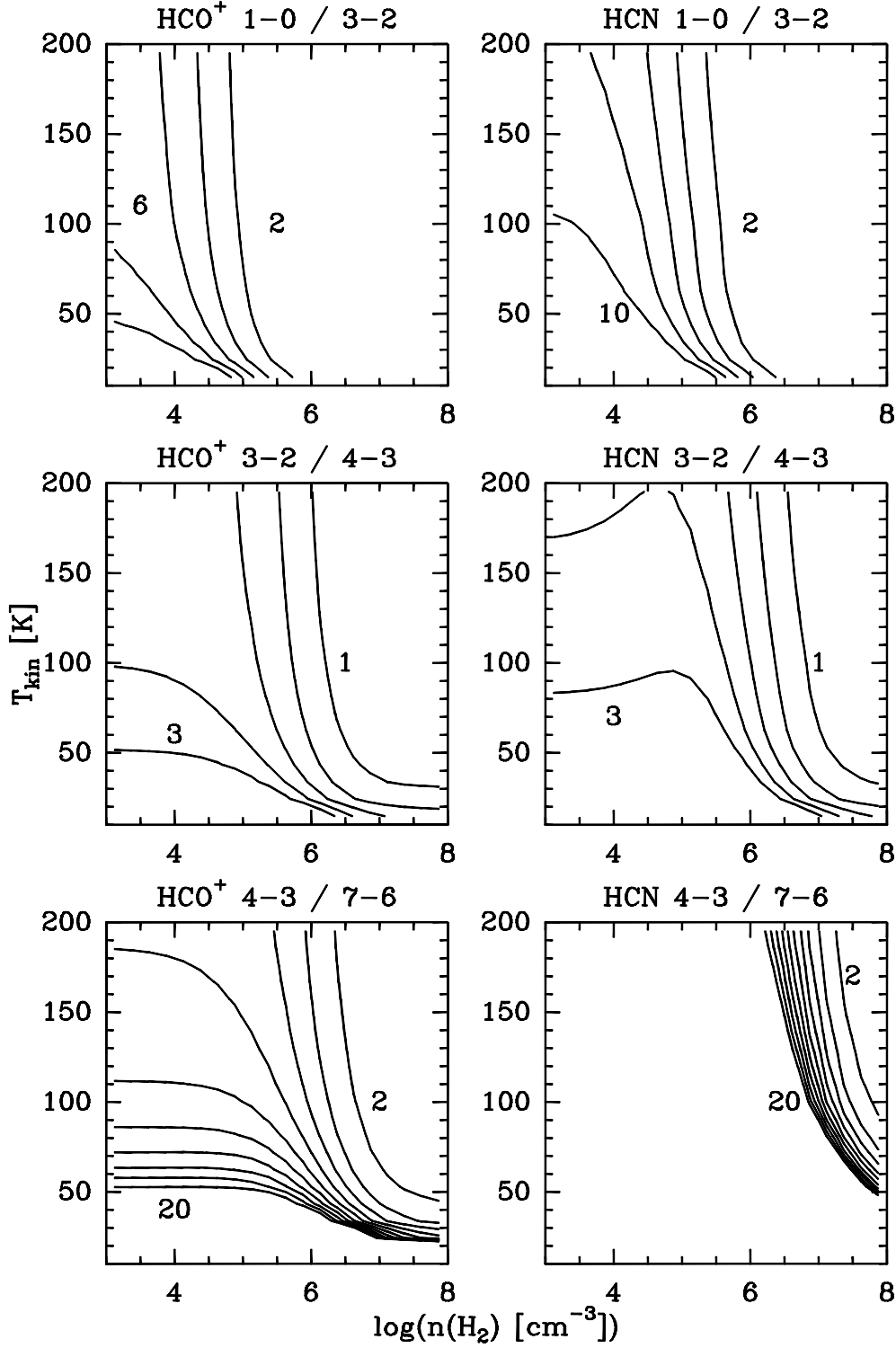
Calculation of rate coefficients is a highly specialized and time consuming effort. New results appear in the literature at a rate of a few molecules per year, which is at or below the detection rate of new interstellar molecules. The point where CRCs are known for all interstellar molecules may thus never be reached. In order to make the best possible use of scarce human and computational resources, we have selected those molecules for which the calculation of new CRCs would have the most astrophysical impact.

The main criterion to assign high priority to a molecule is its importance in constraining astrophysical or astrochemical parameters beyond its own abundance. Calculation of CRCs is most useful for species which uniquely trace certain physics in a wide variety of astrophysical objects.

As a second criterion, the possibility to use old results or results from other molecules is considered. Although direct calculations are always preferred over approximate scalings, the impact of new calculations is somewhat less if scaling may be expected to yield fairly accurate approximations. The most common examples of such scalings are isotopologues, where CRC scaling will only work if the symmetry of the molecule is unchanged (e.g.,  $\text{HCO}^+ \rightarrow \text{DCO}^+$  will work but  $\text{H}_2\text{CO} \rightarrow \text{HD}\text{CO}$  will not); isomers, where scaling only works if the species have similar dipole moments (e.g.,  $\text{HCN} \rightarrow \text{HNC}$  works better than  $\text{HCO}^+ \rightarrow \text{HOC}^+$ ); and O  $\rightarrow$  S substitutions (e.g.,  $\text{H}_2\text{CO} \rightarrow \text{H}_2\text{CS}$ ). Unlike in molecular physics, accuracy to order of magnitude is often enough in astrophysics, and relative rates are more important than absolute values.

The astrophysically most important molecules without any known rate coefficients and without structurally similar species with known rates are:

1. CN is a key tracer of energetic radiation in protoplanetary disks, Galactic PDRs and extragalactic systems es-



**Fig. 1** Line ratios of  $\text{HCO}^+$  and HCN, calculated with RADEX in the optically thin limit as a function of kinetic temperature and  $\text{H}_2$  volume density. Contours are spaced linearly and some contours are labeled for easy identification.

- pecially when compared with HCN (Meijerink & Spaans 2005). Rate coefficients for electron collisions are known (Black & van Dishoeck 1991), but no values for H<sub>2</sub> or He exist. Scaling from CO or CS fails because CN has a  $^2\Sigma$  ground state. Note that calculated rates may be scalable to CO<sup>+</sup>, another tracer of high-energy radiation, recently detected in the active galaxy M 82 (Fuentes et al. 2006).
2. **H<sub>2</sub>D<sup>+</sup> and D<sub>2</sub>H<sup>+</sup>** are unique chemical and kinematic tracers of the centers of pre-stellar cores, where all CNO-bearing species are frozen out on dust grains (Caselli et al. 2003; Van der Tak et al. 2005; Vastel et al. 2004). The asymmetric light-weight structure prevents scaling from other molecules.
  3. **NO** is another readily observed important PDR and XDR tracer. Information from other  $^2\Pi$  molecules such as OH cannot be scaled because of the different Hund case. Experimental cross sections have been measured by the group of Milliard Alexander in Maryland, and may be used as a starting point. The rates may be further scaled to NS, a possible shock tracer (Hatchell & Viti 2002).
  4. **H<sub>3</sub>O<sup>+</sup>** is important as tracer of H<sub>2</sub>O and of the local ionization rate (van der Tak et al. 2006). So far, scaled NH<sub>3</sub> rates have been used (Phillips et al. 1992) which are at best correct to order of magnitude.

Finally it would be useful to develop approximations to derive rate coefficients for large molecules ( $\gtrsim 7$  atoms) for which detailed calculations would take prohibitive amounts of time.

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